where

$$S(z) = \sum_l A_l \cos 2\pi lz, \qquad (2)$$

$z_m$ is the value of $z$ for which $S(z)$ attains its maximum value, and $A_l$ is the $l$th Fourier coefficient. [In the present application $A_l$ is either $\Delta_0(**l)$ itself or $\Delta_0(**l)$ multiplied by the relative areas of cross section given in Table 1.] For two of the 'apatites' $z_m$ is about 0·20, and for the other three it is 0·25. One has, after differentiation and some reduction:

$$\frac{\partial P(z)}{\partial A_l} = S_m^{-1}[\cos 2\pi lz - P(z)\cos 2\pi lz_m], \qquad (3)$$

so that, to the usual approximation,

$$\sigma^2[P(z)] = S_m^{-2}\sum_l[\cos 2\pi lz - P(z)\cos 2\pi lz_m]^2\sigma^2(A_l). \qquad (4)$$

The variance of $P(z)$ thus vanishes, as obviously it should, for $z = z_m$, and varies slowly but appreciably with $z$ over the rest of the range. The error bars attached to the curve for $Cd_5(VO_4)_3$ in Fig. 1 correspond to ±3$\sigma$, the standard deviations of $\Delta_0(**l)$ being taken from Table 1 of Wilson, Sudarsanan & Young (1977).

## Discussion

Not surprisingly, the intuitive deduction about the behaviour of Fourier syntheses, based on analogy with results in particle-size broadening (Wilson, 1979, §2.7.2), is confirmed by calculation.

Wilson, Sudarsanan & Young (1977) compared their values of $\Delta_0(**l)$ with those to be expected for a uniform distribution (square wave.). This function was chosen partly because of its simplicity, partly because other models (Gaussian, Cauchy, Laplacian) were excluded by the behaviour of the signs of $\Delta_0(**l)$, and partly because the dip in the distribution functions for two 'apatites' at $z = 0{\cdot}25$ was reminiscent of that given by a square wave represented by only its first few Fourier components. It is therefore of interest to calculate what a square wave would look like if synthesized from its first seven Fourier coefficients, seven being the maximum number available for any of the 'apatites' (even values of $l$ up to 14). Such a curve is shown in Fig. 1 for a square wave with half-width $\delta$ approximately the expected value for $Cd_5(VO_4)_3I$. The 'observed' distribution for this substance lies below the square wave by much more than 3$\sigma$ near $z = 0{\cdot}12$, as would be expected from the weakness of the $\Delta_0(**4)$ component, noted for four of the five substances in the earlier paper.

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*Acta Cryst.* (1981). A**37**, 442–443

# On the occurrence of polytypism in cadmium sulphide thin films.

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(*Received* 15 *December* 1978; *accepted* 19 *November* 1980)

## Abstract

Cadmium sulphide thin films have been found to exhibit the occurrence of polytypism. The polytypes are formed when amorphous cadmium sulphide thin films undergo an amorphous to crystalline transformation. The single-crystal regions correspond to different polytypes. Two types of polytypic modifications were found to occur most frequently. One of these, the low-temperature modification, had $a = 4{\cdot}15$ and $c = 6{\cdot}72$ Å and corresponded to the known crystallographic variant $2H$. The observed polytypes based on this phase were $4H$ ($a = 4{\cdot}15$; $c = 13{\cdot}44$ Å) and $6H$ ($a = 4{\cdot}15$; $c = 20{\cdot}16$ Å). In addition, a disordered long-period polytype has also been observed. The other common type found was a high-temperature modification with $a = 5{\cdot}12$ and $c = 8{\cdot}62$ Å. This new type has been designated as $2H_1$. The observed polytype based on this modification corresponded to $5H_1$ ($a = 5{\cdot}12$; $c = 21{\cdot}50$ Å).

Cadmium sulphide is an important electronic semiconductor (band gap 2·5 eV) and has recently been widely used in the fabrication of solar cells. Although it is isostructural with zinc sulphide, which exhibits a profuse preponderance of polytypes, until recently no polytype except $2H$ had been found to occur in cadmium sulphide (Baronnet, 1978). In view of the facts that the electronic band gap of the polytypic crystals varies with polytype periodicity (Knippenberg, 1963; Rao & Srivastava, 1978) and that for maximum efficiency of energy conversion in solar cells there is an optimum band gap of about 1·5 eV (Loferski, 1950), there is some justification in studies seeking to explore the possibility of occurrence of polytypism in cadmium sulphide. We have recently found that in sharp contrast to the known results on single crystals and polycrystalline structural variants (both in bulk and thin-film form) polytypes do form in their single-crystal regions as a consequence of amorphous CdS films transforming to the crystalline phase. Besides the known $2H$ and $3C$ phases several new polytypes such as $4H$, $6H$, $2H_1$ and $5H_1$ have been found to be formed in the present investigation. Here the subscript 1 denotes a new hexagonal phase whose lattice parameters are different from that of $2H$, and $5H_1$ is a polytype based on $2H_1$.

Amorphous CdS thin films were formed by depositing

0567-7394/81/030442-02$01.00

electronic grade CdS by thermal evaporation under vacuum ($1\cdot3 \times 10^{-4}$ Pa) on glass slides which were precooled to liquid-nitrogen temperature. The films employed in the present investigation had thicknesses ranging from 200 to 700 Å. The crystallographic characterization was done by employing electron microscope techniques – in both imaging and diffraction modes. It was found that the initial phase of the film was amorphous. On undergoing an amorphous to crystalline transformation brought about by annealing the amorphous films up to a temperature of about 773 K by employing a focused electron beam for 10 to 30 s, single-crystal regions were formed. The annealing temperature was ascertained from a precalibration of the electron beam (Srivastava & Srivastava, 1975). After cooling the sample almost to room temperature the diffraction patterns were recorded from the single-crystal regions. The diffraction pattern which was most often observed corresponded to a hexagonal phase with $a = 4\cdot15$ and $c = 6\cdot72$ Å. This is compatible with the known $2H$ phase. Although the electron diffraction intensities are not very accurate, intensity data collected from several patterns suggested that this phase has the known wurtzite-type structure. Very often diffraction patterns were found which were unequivocally explicable based on the same periodicity in the $a$ direction as that of $2H$ but with the periodicity in the direction of $c$ being double and triple that of $2H$, *i.e.* $c = 13\cdot44$ and $c = 20\cdot16$ Å. Thus, apart from $2H$, the polytypes $4H$ and $6H$ were also stabilized as a consequence of the amorphous to crystalline transformations. Besides these, some other polytypes with high periodicity whose identity could not be definitely established were also obtained. The determination of the stacking sequence (structure) for none of these polytypes was attempted. The foregoing polytypes, when once formed, did not transform to any other structure on annealing at high temperatures and thus they represented stable phases.

In order to explore the high-temperature transformation characteristics of the initial amorphous films, annealing was also done at high temperatures $773 \leq T \leq 1173$ K. This mode of annealing was found to yield two different modifications: both of these were hexagonal and had the same periodicity along **a** ($a = 5\cdot12$ Å). The periodicities along **c** were 8·62 and 21·50 Å. The most commonly occurring modification (high-temperature modification) was the one with $c = 8\cdot62$ Å. Taking this to correspond to the phase with the minimum number of layers in the unit cell, it can be designated as $2H_1$. The other modification is $5H_1$. Some other polytypes in this category were disordered. Preliminary observations carried out by us on other cadmium chalcogenides revealed that the occurrence of polytypism in thin films is a general phenomenon. Thus, when amorphous cadmium telluride thin films transform to the crystalline phase, several polytypes are found to result.

In conclusion, it can be said that several new polytypes have been found to exist in cadmium sulphide thin crystals. These represent the first reported polytypes of cadmium sulphide. As regards the mechanism of formation, in view of the special mode of stabilization of polytypes, as a consequence of amorphous to crystalline transformation, none of the known mechanisms (Baronnet, 1978) can directly explain the genesis of CdS polytypes. It appears that a new possible mechanism will have to be worked out to make the formation of the present polytypes intelligible. Attempts are being presently made to put forward a feasible mechanism and results will be forthcoming.

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# International Union of Crystallography

*Acta Cryst.* (1981). A**37**, 443–444

## Commission on Journals

### Standards for the Publication of Powder Pattern Data

Standards for the publication of powder patterns, originally compiled by a subcommittee of the American Crystallographic Association and published in *National Bureau of Standards Special Publication* 567 (1979), have been accepted by the Commission on Crystallographic Data and the Commission on Journals. Papers that present powder pattern data submitted for publication in IUCr journals are now required to follow these standards.

The information requested by the standard data-form, a completed example of which is given in Table 1, must be given as compactly as possible. Essential information is requested by the bold-face headings. The remaining information sought is highly desirable, although it is recognized that some may not be available in all cases. Partial omission of the optional data will not preclude publication of the paper. Powder data corresponding to the information given in Table 1 are presented, in the preferred form, in Table 2. Reprints of the complete standard, including copies of the blank data-form, are available from any Co-editor. Guidance in filling out the form is available from the JCPDS International Center for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, USA.

Among the requirements for reporting powder diffraction data are:

(*a*) The published powder pattern should be as complete as possible and should include weak as well as strong diffraction lines. Where possible, the data should extend to at least 100° $2\theta$ (Cu $K\alpha$ radiation). Patterns with a small number of lines should extend to the limit of the experimental method used.

(*b*) The experimentally observed $2\theta$ values should be given in degrees, corrected for systematic instrumental error.

(*c*) Intensities should be reported numerically, with the most intense line scaled to 100 and intensities less than 1 reported